L16 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2007:898276 CAPLUS <<LOGINID::20080331>> DOCUMENT NUMBER: 147:437252 TITLE: Supramolecular crystal structures of per(3,6- $\underline{\text{anhydro}}) - \alpha - \underline{\text{cyclodextrin}}$ grown from KCl or NaI solutions AUTHOR(S): Baudin, Cecile; Camara, Magatte; Navaza, Alda CORPORATE SOURCE: DRECAM/LSI, CEA, CEA Saclay, Gif-sur-Yvette, F-91191, SOURCE: Journal of Molecular Structure (2007), 839(1-3), 58-63 CODEN: JMOSB4; ISSN: 0022-2860 PUBLISHER: Elsevier B.V. DOCUMENT TYPE: Journal LANGUAGE: English Crystals of per(3,6-anhydro)- α - cyclodextrin {hexakis(3,6-anhydro)cyclomaltohexaose} (1) grown in presence of KCl or NaI evidence the similar distorted conformation of macrocycle and provide the same supramol. scaffolding of cyclodextrins based on CH•••O H bonds. Infinite tubes parallel to symmetry axis 6 are filled by H2O mols. or by I atoms in 1/KCl and 1/NaI crystals, resp. In 1/KCl crystals an inclusion complex of stoichiometry 1:2 was found. Coordination polyhedra of the dimeric K units fuse with the coordination polyhedra of one pentacoordinated chloride atom to form an infinite helixalong the c direction crossing over a helical organic envelope of cyclodextrin mols. Crystallog. data are given. REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT L16 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2007:724927 CAPLUS <<LOGINID::20080331>> DOCUMENT NUMBER: 147:277817 TITLE: NMR spectroscopy on the complexation of 3,6anhydro- β - cyclodextrin with 2,6-naphthalene-dicarboxylate ion AUTHOR(S): Yoshikiyo, Keisuke; Matsui, Yoshihisa; Yamamoto, Tatsuyuki; Okabe, Yuji Faculty of Life and Environmental Science, Shimane CORPORATE SOURCE: University, 1060 Nishikawatsu, Matsue, 690-8504, Japan Bulletin of the Chemical Society of Japan (2007), SOURCE: 80(6), 1124-1128 CODEN: BCSJA8; ISSN: 0009-2673 PUBLISHER: Chemical Society of Japan DOCUMENT TYPE: Journal LANGUAGE: English The 2,6-naphthalene-dicarboxylate ion (2,6-NDC) was included into the interior cavity of 3A,6A-anhydro- β - cyclodextrin (I) in D2O containing 0.1 mol dm-3 Na2CO3 and caused a shift in the 1H NMR signals due to the C3- and C5-H's of I to different directions, depending on the positions of glucose units (anisotropic ring-current effect). The decrease in entropy accompanied by the complexation was much larger than that for the complexation of native $\beta\text{--}$ cyclodextrin with 2,6-NDC. These results indicate that the mol. rotation of 2,6-NDC is retarded within the deformed cavity of I. REFERENCE COUNT: THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS 1.0 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT L16 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2005:10691 CAPLUS <<LOGINID::20080331>> DOCUMENT NUMBER: 142:280362 TITLE: Ionic complexation properties of per(3,6- $\underline{\text{anhydro}})\,\underline{\text{cyclodextri}\underline{n}}\ \text{derivatives}$ towards lanthanides Baudin, Cecile; Tardy, Fabienne; Dalbiez, Jean-Pierre; AUTHOR(S): Jankowski, Christophe; Fajolles, Christophe; Leclair, Gaetan; Amekraz, Badia; Perly, Bruno; Mauclaire, Laurent CEA, DRECAM/SCM, CEA Saclay, Gif-sur-Yvette, F-91191, CORPORATE SOURCE: Fr. Carbohydrate Research (2005), 340(1), 131-138 SOURCE:

CODEN: CRBRAT; ISSN: 0008-6215

Elsevier B.V.

PUBLISHER:

```
LANGUAGE:
                          English
                         CASREACT 142:280362
OTHER SOURCE(S):
     Using per(3,6-anhydro)cyclodextrin derivs. [per(3,6-anhydro)CD], it was possible to produce new lanthanide, such as
     praseodymium, chelates by careful choice of the size and functional
     groups. Heptakis(3,6-<u>anhydro</u>-2-0-methyl)cyclomaltoheptaose
     fulfills the best criteria for complexation of praseodymium ions. NMR was
     used to derive the association consts. and the stoichiometries of these new
     complexes. Finally, a three-dimensional structure of these complexes
     consistent with the NMR data is proposed, to ascertain the position of
     praseodymium in the cavity of the per(3,6-anhydro)CD. For the
     present purposes, heptakis(2-0-acetyl-3,6-anhydro
     )cyclomaltoheptaose, octakis(2-0-acetyl-3,6-anhydro
     )cyclomaltooctaose, heptakis(3,6-anhydro-2-0-
     methyl)cyclomaltoheptaose and octakis(3,6-anhydro
     -2-0-methyl)cyclomaltooctaose have been synthesized and purified.
                                THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS
REFERENCE COUNT:
                          35
                                RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
L16 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2008 ACS on STN
                          1998:172422 CAPLUS <<LOGINID::20080331>>
ACCESSION NUMBER:
DOCUMENT NUMBER:
                          128:283005
                          Primary hydroxy-modified cyclomaltoheptaose
TITLE:
                          derivatives with two kinds of substituents.
                          Preparation of 6I-(benzyloxycarbonylamino)-,
                          6I-(tert-butoxycarbonylamino)- and
                          6I-azido-6I-deoxy-6II,6III,6IV, 6V,6VI,6VII-hexa-0-
                          tosylcyclomaltoheptaose and their conversion to the
                          hexakis-(3,6-<u>anhydro</u>) derivatives
AUTHOR(S):
                          Yamamura, Hatsuo; Yotsuya, Tadahiro; Usami, Satoshi;
                          Iwasa, Akihito; Ono, Shoji; Tanabe, Yoshihisa; Iida,
                          Daisuke; Katsuhara, Takao; Kano, Kazuaki; Uchida,
                          Tetsuo; Araki, Shuki; Kawai, Masao
                          Department of Applied Chemistry, Nagoya Institute of
CORPORATE SOURCE:
                          Technology, Nagoya, 466, Japan
SOURCE:
                          Journal of the Chemical Society, Perkin Transactions
                          1: Organic and Bio-Organic Chemistry (1998), (7),
                          1299-1304
                          CODEN: JCPRB4; ISSN: 0300-922X
PUBLISHER:
                          Royal Society of Chemistry
DOCUMENT TYPE:
                          Journal
LANGUAGE:
                          Enalish
    Three cyclomaltoheptaoses (1, 2 and 3) which possess a
     benzyloxycarbonylamino group, a tert-butoxycarbonylamino group or an azido
     group, and six tosyloxy groups, on their C-6 atoms have been prepared These
     can be versatile intermediates for the synthesis of derivs. possessing an
     amino group as well as other functional groups. As an example of their
     derivatization, their conversion to compds. containing 3,6-anhydroglucoses,
     which possess cation-binding abilities, is also reported.
                                THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS
REFERENCE COUNT:
                          22
                                RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
L16 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:
                         1996:733917 CAPLUS <<LOGINID::20080331>>
DOCUMENT NUMBER:
                          126:25956
TITLE:
                          Dipotassium Complex of Per-3,6-anhydro
                          -β- cyclodextrin
Ashton, Peter R.; Gattuso, Giuseppe; Koeniger, Rainer;
AUTHOR(S):
                          Stoddart, J. Fraser; Williams, David J.
CORPORATE SOURCE:
                          School of Chemistry, University of Birmingham,
                          Edgbaston/Birmingham, B15 2TT, UK
                          Journal of Organic Chemistry (1996), 61(26), 9553-9555
SOURCE:
                          CODEN: JOCEAH; ISSN: 0022-3263
                          American Chemical Society
PUBLISHER:
DOCUMENT TYPE:
                          Journal
LANGUAGE:
                          English
     The complete 3,6-anhydration of <u>cyclodextrins</u> induces severe changes into the conformations of the D-glucopyranose residues, imposing a
     1C4 chair conformation in contrast with the usual 4C1 chair. Mass
     spectrometric evidence is presented, which shows that per-3,6-
     \underline{\text{anhydro}} \neg \beta \neg \ \underline{\text{cyclodextrin}} \ \text{complexes} \ \text{K ions selectively}
```

DOCUMENT TYPE:

Journal

from a melee of alkali metal cations. X-ray crystallog. anal. reveals that, in the solid state, the highly distorted chemical-modified cyclodextrin adopts a severely puckered conformation, which facilitates the binding of two K ions with the cavity of per-3,6anhydro- β - cyclodextrin. These cations, which are 10- and 11-coordinate, bind to 0 atoms, other than the anhydro ring O atoms, in six (two only partially) of the seven 3,6-anhydro -D-glucopyranose residues. Included H2O mols. and/or HO- ions serve to satisfy the remaining coordination sites. Study of the crystal packing reveals that the 2:1 complexes assemble to form a trimeric C3 sym. clover leaf aggregate.

L16 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1995:909459 CAPLUS <<LOGINID::20080331>>

DOCUMENT NUMBER: 123:290262

TITLE: Manufacture method and use of mono-3,6-anhydro

-cyclodextrins for solubilizing hydrophobic compound and monitoring the purity of enantiomer

INVENTOR(S): Djedaini-Pilard, Florence; Perly, Bruno PATENT ASSIGNEE(S): Commissariat a l'Energie Atomique, Fr.

SOURCE: PCT Int. Appl., 24 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: French FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA	PATENT NO.					KIND		DATE		APPLICATION NO.					DATE		
MO	9517	433			A1		19950629			WO	√0 1994-FR1502					19941221	
	W:	ΑU,	HU,	JP,	US												
	RW:	ΑT,	BE,	CH,	DE,	DK	, ES,	FR,	GB,	GF	R, IE,	ΙT,	LU,	MC,	NI	L, PT,	SE
FR	2714	066			A1		1995	0623		FR	1993-	1547	0			199312	222
FR	2714	066			В1		1996	0112									
AU	9513199				A		1995	0710		ΑU	1995-	1319	9			199412	221
AU	6879	66			В2		1998	0305									
EP	736045				A1		1996	1009		EP	1995-	9045	78			199412	221
EP	736045				В1		19990317										
	R:	CH,	DE,	GB,	ΙT,	LΙ	, NL,	SE									
HU	7494	0			A2		1997	0328		HU	1996-	1735				199412	221
HU	2198	80			В		2001	0828									
JP	09506921			T		1997	0708		JP	1995-	5172	34			199412	221	
JP	3604390			В2		20041222											
US	5760	016			A		1998	0602		US	1996-	6524	67			199612	209
PRIORIT:	IORITY APPLN. INFO.:									FR	1993-	1547	0	I	A	199312	222
										WO	1994-	FR15	02	V	V	199412	221

MARPAT 123:290262 The title compds. having good solubility in water and ring size corresponding to $\alpha\text{--},\ \beta\text{--}$ and $\gamma\text{--}$ cyclodextrin are useful for formation of inclusion complexes with hydrophobic compds. for cosmetic formulation, pharmaceuticals, etc. and are prepared by the reaction of a C6-monotosylated cyclodextrin with an aqueous LiOH solution followed by

L16 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1994:192120 CAPLUS <<LOGINID::20080331>>

DOCUMENT NUMBER: 120:192120

regular working up steps.

Conformational study of 3A,6A-anhydro TITLE:

-cyclomaltohexaose in solution

AUTHOR(S): Durier, Viviane; Mazeau, Karim; Gey, Claude; Driguez,

Hugues; Taravel, Francois R.

Cent. Rech. Macromol. Veg., CNRS, Grenoble, 38041, Fr. New Journal of Chemistry (1993), 17(12), 843-9 CORPORATE SOURCE:

SOURCE:

CODEN: NJCHE5; ISSN: 1144-0546

DOCUMENT TYPE: Journal LANGUAGE: English

The conformational behavior of a modified cyclodextrin,

3A,6A-anhydrocyclomaltohexaose in solution, and of two model disaccharides

(Me 4-0- $(\alpha$ -D-glucopyranosyl)-3,6- anhydro $-\beta$ -D-glucopyranoside, and Me 4-0-(3,6- anhydro

 $-\alpha$ -D-glucopyranosyl)- β -D-glucopyranoside) has been

characterized through combined NMR and mol. modeling studies. In

parallel, the conformational anal. of the disaccharides and of the modified cyclodextrin was achieved with the CHARMM program. Both disaccharides have limited stability (ϕ, ψ) domains because of steric repulsions, lack of flexibility of the 3,6-anhydro unit, and the existence of several inter-residue hydrogen bonds. The agreement between exptl. and calculated vicinal coupling consts. is good. Generated conformations for the modified cyclodextrin, have been classified into three groups: regular, intermediate and distorted. For the latter, a glucose unit adjacent to the $3,6-\underline{anhydro}$ residue is tilted towards the inside of the hydrophobic cavity. The NMR data are in agreement with the data calculated for the intermediate form which could correspond to the preferred conformation in solution

L16 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1992:21341 CAPLUS <<LOGINID::20080331>>

DOCUMENT NUMBER: 116:21341

TITLE: Synthesis and characterization of per-3,6-

anhydro cyclodextrins Ellwood, P.; Stoddart, J. F. AUTHOR(S):

CORPORATE SOURCE: Dep. Chem., Univ. Sheffield, Sheffield, S3 7HF, UK SOURCE: Minutes Int. Symp. Cyclodextrins, 5th (1990), 86-9.

Editor(s): Duchene, Dominique. Ed. Sante: Paris, Fr.

CODEN: 57LSAJ

DOCUMENT TYPE: Conference LANGUAGE: English

A symposium on the synthesis and characterization of a potentially new class of cyclodextrin (CD)-derived mol. receptors, the per-3,6anhydro CDs. The $\beta-\text{CD}$ derivative was prepared by treatment of per-6-0-tosyl- β -CD with aqueous NaOH. The per-3,6-anhydride of lpha-CD, however, was prepared by the action of aqueous NaOH on per-6-0-tosyl-2,3-benzoyl- $\!\alpha\text{-CD}$ as the key intermediate.

L16 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1991:82320 CAPLUS <<LOGINID::20080331>>

DOCUMENT NUMBER: 114:82320

TITLE: Synthesis and characterization of per(3,6-

anhydro) cyclodextrins

Ashton, Peter R.; Ellwood, Paul; Staton, Ian; AUTHOR(S):

Stoddart, J. Fraser

CORPORATE SOURCE: Dep. Chem., Univ. Sheffield, Sheffield, S3 7HF, UK Angewandte Chemie (1991), 103(1), 96-7 (See also SOURCE:

Angew. Chem., Int. Ed. Engl., 1991, 30(1), 80-1)

CODEN: ANCEAD; ISSN: 0044-8249

DOCUMENT TYPE: Journal LANGUAGE: German

The title compds. were prepared via treatment of 6-0-tosylcyclodextrins with aqueous NaOH or their perbenzoates with Et3N in aqueous MeOH. The crystal

structure of anhydro- β - cyclodextrin was determined